

Hybrid Crystals of Cuprates and Iron-Based Superconductors

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We propose two possible new compounds, $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ and $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$, which hybridize the building blocks of two high temperature superconductors, cuprates and iron-based superconductors. These compounds consist of square CuO_2 layers and antiferrotype-type Fe_2X_2 ($\text{X}=\text{As}, \text{Se}$) layers separated by Ba/K. The calculations of binding energies and phonon spectrums indicate that they are dynamically stable, which ensures that they may be experimentally synthesized. The Fermi surfaces and electronic structures of the two compounds inherit the characteristics of both cuprates and iron-based superconductors. These compounds can be superconductors with intriguing physical properties to help to determine pairing mechanisms of high T_c superconductivity.

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I. INTRODUCTION

Cuprates¹⁻⁸, first discovered in 1986, and iron-based superconductors⁹⁻¹³ (IBS), discovered in early 2008, are two classes of unconventional high temperature superconductors who share many common features. Both of them are quasi-two-dimensional and the phase diagrams are similar in which superconductivity develops after a magnetic order is suppressed¹⁴⁻¹⁶. All the cuprates share a common structure element CuO_2 plane, where Cu atoms form a square lattice¹⁷. The IBS share a common Fe_2X_2 ($\text{X}=\text{As}$ and Se) layered structure unit, which possesses an anti-PbO-type (anti-litharge-type) atom arrangement. The Fe_2X_2 layers consist of a square lattice sheet of Fe coordinated by X above and below the plane to form face sharing FeX_4 tetrahedra¹⁸.

One of major questions in the field of high T_c superconductors is whether cuprates and IBS share a common superconducting mechanism^{16,19}. The answer to this question may be obtained if we can integrate the characteristics of both superconductors into a single compound so that their relations can be exclusively addressed. As both structures are featured with layered square lattices with similar in-plane lattice constants, it is possible to design a compound containing both building blocks, Cu-O layers of cuprates and Fe-As(Se) layers of IBS. A similar material design has been adopted and a target material $\text{Nd}_4\text{CuO}_6\text{Fe}_2\text{As}_2$ has been theoretically investigated²⁰.

Recently, two new materials $\text{Ba}_2\text{MO}_2\text{Ag}_2\text{Se}_2$ ($\text{M} = \text{Co}, \text{Mn}$)²¹ have been synthesized via solid-state reaction in experiment. These two compounds, whose structures belong to I4/mmm space group, consist of infinite MO_2 square planes and antiferrotype-type Ag_2Se_2 layers separated by barium. In this paper, motivated by the fact that the MO_2 plane resembles the CuO_2 plane in cuprates and the Ag_2Se_2 layer resembles the Fe_2X_2 layer in IBS, we consider the substitution of Cu and Fe for M and Ag in the compounds respectively to obtain two possible new compounds, $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ and $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$. We perform density functional calculations to study the stability and basic electronic structures of these new compounds. We find that these materials integrate basic electronic characteristics of both high T_c superconductors. In

$\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$, the CuO_2 layers are electron-doped while the Fe_2As_2 layers are hole-doped. The situation is reversed in $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$. Such doping configurations suggest that many possible mixed phases, in particular, magnetic and superconducting phases, may be realized in these materials by introducing additional carriers and applying external pressure.

II. COMPUTATIONAL DETAILS

Our calculations are performed using density functional theory (DFT) employing the projector augmented wave (PAW) method encoded in the Vienna ab initio simulation package (VASP)²²⁻²⁴. Both of the local density approximation (LDA) and generalized-gradient approximation (GGA)²⁵ for the exchange correlation functional are used. Throughout the work, the cutoff energy is set to be 500 eV for expanding the wave functions into plane-wave basis. In the calculations of magnetic properties, the LDA+U method is used with the effective on-site Coulomb U being 7 eV for Cu 3d states²⁶. In the calculations, the Brillouin zone is sampled in the \mathbf{k} space within Monkhorst-Pack scheme²⁷. The number of these k points are depending on the lattice: $15 \times 15 \times 3$ for the general unit cell with 4 Fe atoms and 2 Cu atoms and $9 \times 9 \times 3$ for the $\sqrt{2} \times \sqrt{2}$ unit cell. We relax the lattice constants and internal atomic positions with both LDA and GGA, where forces are minimized to less than 0.01 eV/Å. The phonon dispersions are calculated using finite displacement method²⁸ as implemented in the PHONOPY code^{29,30}.

III. CRYSTAL STRUCTURE

$\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ and $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$ crystallize in a body-centered tetragonal lattice, shown in Figure 1. The Ba (K) spacer layer separates the tetrahedra Fe_2As_2 (Fe_2Se_2) layers and the square CuO_2 layers. There are double Fe_2X_2 ($\text{X}=\text{As}$ and Se) and CuO_2 layers in a unit cell, similar to BaFe_2As_2 . In order to predict the structures of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ and $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$, the lattices are fully optimized based on the

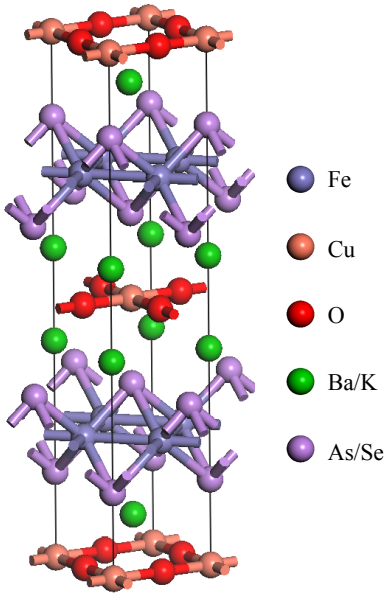


FIG. 1: (color online) Crystal structure of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ ($\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$).

experimental structural parameters of $\text{Ba}_2\text{CoO}_2\text{Ag}_2\text{Se}_2$. The optimized and experimental structural parameters are summarized in Table I. Both of the calculated lattice constants using LDA and GGA are close to those of $\text{Ba}_2\text{CoO}_2\text{Ag}_2\text{Se}_2$ in experiment, which validates the adopted substitution. As the calculated lattice parameters for $\text{Ba}_2\text{CoO}_2\text{Ag}_2\text{Se}_2$ using GGA are closer to the experimental data, we perform the following calculations for the two materials using the lattice parameters obtained by relaxation with GGA.

The binding energy is usually calculated to estimate the stability of new structures. Here, the binding energy per atom, E_b , is defined as $E_b = (4E_{\text{Ba/K}} + 2E_{\text{Cu}} + 4E_{\text{O}} + 4E_{\text{Fe}} + 4E_{\text{As/Se}} - E_{\text{total}})/18$, in which $E_{\text{Ba}}, E_{\text{K}}, E_{\text{Cu}}, E_{\text{O}}, E_{\text{Fe}}, E_{\text{As}}$ and E_{Se} are the respective energies per atom of elemental Ba, K, Cu, O, Fe, As and Se in the states at standard ambient temperature and pressure. E_{total} is the calculated total energy of a unit cell of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ ($\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$). The obtained binding energies are 1.61 eV and 1.23 eV per atom for $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ and $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$, respectively. Both of the binding energies are very close to that of $\text{Ba}_2\text{CoO}_2\text{Ag}_2\text{Se}_2$ (1.318 eV), indicating that the two structures are energetically favorable in experiment and may be synthesized using similar methods. To further test the stability of these two structures, we calculate their phonon dispersions, shown in Figure 2. No imaginary frequencies are observed throughout the whole Brillouin zone in phonon dispersions, confirming their dynamically structural stability.

IV. ELECTRONIC AND MAGNETIC PROPERTIES

The optimized parameter a of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ is determined to be 4.026 Å, slightly bigger than those of cuprates (3.78 Å for $\text{La}_{1.8}\text{Sr}_{0.2}\text{CuO}_4$ ³ and 3.859 Å for

TABLE I: Optimized structural parameters of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ and $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$, using LDA and GGA in the paramagnetic phase. The 6th column is the experimental structural parameters of $\text{Ba}_2\text{CoO}_2\text{Ag}_2\text{Se}_2$ ²¹.

	$\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$		$\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$		$\text{Ba}_2\text{CoO}_2\text{Ag}_2\text{Se}_2$
	LDA	GGA	LDA	GGA	Expt.
$a(\text{\AA})$	3.902	4.026	3.769	3.839	4.223
$c(\text{\AA})$	19.867	20.273	18.320	22.165	20.036

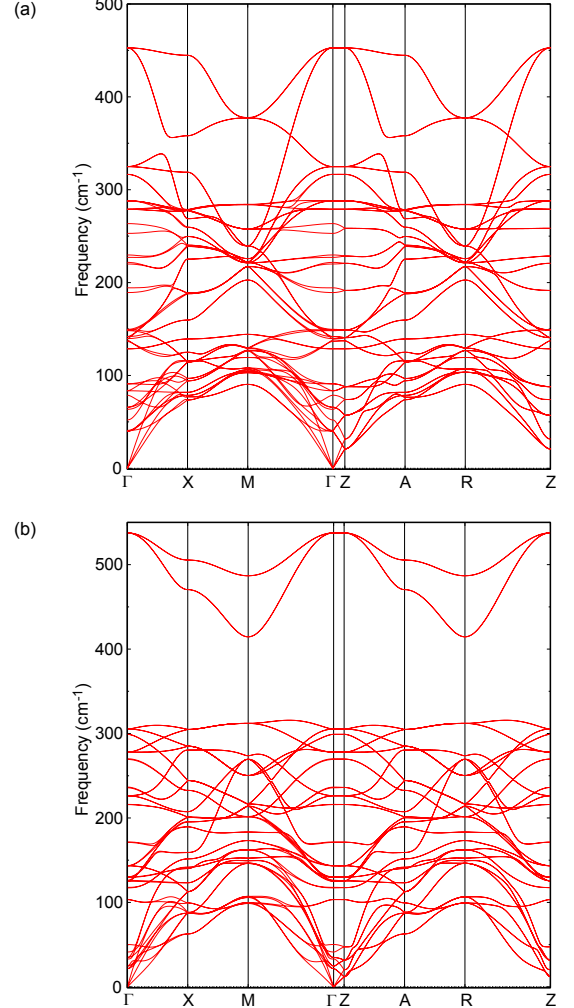


FIG. 2: (color online) Calculated GGA phonon dispersions of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ and $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$ in the paramagnetic state.

TABLE II: Optimized structural parameters of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ using GGA in the paramagnetic phases and those of LiFeAs ¹⁰, BaFe_2As_2 ¹¹ and LaFeAsO ⁹. The angle β is the Fe-As-Fe bonding angle of two next nearest Fe atoms.

	$\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$	LiFeAs	BaFe_2As_2	LaFeAsO
$a(\text{\AA})$	4.026	3.791	3.963	4.035
$\beta(^{\circ})$	118.7	103.1	111.0	113.5
$h(\text{Fe-As})(\text{\AA})$	1.19	1.51	1.36	1.32
$h(\text{Fe-Fe})(\text{\AA})$	10.14	6.36	6.51	8.74

YBa₂Cu₃O_{6+x}⁴). Compared with three typical kind of iron pnictides, LiFeAs¹⁰, BaFe₂As₂¹¹, and LaFeAsO⁹, as shown in Table II, the parameter a is very close to those of BaFe₂As₂ and LaFeAsO but deviates a little from that of LiFeAs. The obtained As height above the Fe plane in Ba₂CuO₂Fe₂As₂ is smaller than those of iron pnictides in experiment. This underestimation has been noted in the study of IBS^{31–33}. The Fe₂As₂ inter-layer distance is much larger than the values of the three families in iron pnictides, indicating that it is more two-dimensional than conventional iron pnictides. The separation between Fe₂As₂ and CuO₂ layers is about 5 Å, which suggests couplings between these layers.

The band structure and density of states (DOS) for Ba₂CuO₂Fe₂As₂ with GGA optimized structural parameters in the paramagnetic states are shown in Figure 3. The band structure near the Fermi level resembles those of both typical iron pnictides LaFeAsO³⁴ and cuprates¹⁴ where Fe 3d states (d_{xz} , d_{yz} , $d_{x^2-y^2}$ orbitals) and Cu 3d states ($d_{x^2-y^2}$ orbitals) dominate the Fermi level. Similar to iron pnictides, it is a bad metal with low carrier density. The 3d states of Fe are mainly located near the Fermi level from -2.5 eV to 3.0 eV and a pseudogap appears at an electron count of six. The As p states mainly lie 2.5 eV below the Fermi level but slightly mix with the Fe 3d states in the energy range from -1.0 eV to 1.0 eV. The Cu 3d contribution is concentrated between -3.0 eV and 1.5 eV. The O p states are strongly coupled with 3d states of Cu in the total energy range. The spacer layer Ba 5d and 6s states, which donate electrons to Fe₂As₂ and CuO₂ layers, are empty and lie 2 eV above the Fermi level. At the Fermi level, the total DOS shows the same negative slope with the minimum slightly above the Fermi level, similar to the conventional IBS within DFT. The DOS at the Fermi energy is about 7.81 eV⁻¹/f.u. for both spins. Considering that there are two Fe atoms in one formula unit for Ba₂CuO₂Fe₂As₂ but only one for LaFeAsO, this value (3.91 eV⁻¹/Fe) is larger than that of LaFeAsO (2.62 eV⁻¹/f.u.³⁴). The corresponding Pauli susceptibility and specific heat coefficient are $\chi_0 = 2.53 \times 10^{-4}$ emu/mol and $\gamma = 18.4$ mJ/(K² mol).

The calculated Fermi surfaces of Ba₂CuO₂Fe₂As₂ are given in Figure 4, which are very similar to those of both iron pnictides and cuprates. From Figure 3(a), we find that the Fe d_{xz} and d_{yz} states yield two hole cylinders at the zone center. There is an additional heavy 3D hole pocket centered at Γ point, which intersects and anticrosses with the hole cylinders. The 3D pocket is derived from Fe d_{z^2} states which hybridize with As p_z states. At the zone corner, there are two 2D small electron pockets and one 2D large hole pocket. The electron pockets are mainly attributed to Fe d_{xz} , d_{yz} and $d_{x^2-y^2}$ orbitals (d_{xy} orbitals in usual Fe lattice). The hole pocket around M point, however, is mainly derived from Cu $d_{x^2-y^2}$ and O p_x and p_y states, in accordance with the Fermi surfaces of cuprates¹⁴. All of the Fermi surface sheets are double degenerate as there are two Fe₂As₂ and CuO₂ layers in one unit cell.

It is interesting to see that the hole pockets at Γ point are large, which indicates heavy hole doping in the Fe₂As₂ layers. From the size of the pockets, we can estimate that the hole doping concentration with respect to BaFe₂As₂ is roughly

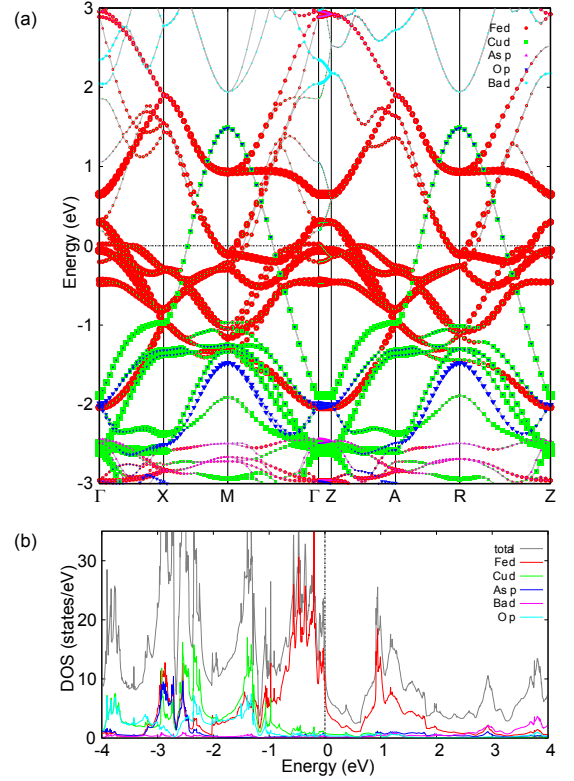


FIG. 3: (color online) Band structures and projected density of states of Ba₂CuO₂Fe₂As₂ using GGA relaxed parameters in the paramagnetic state.

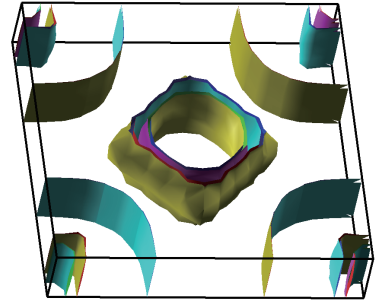


FIG. 4: (color online) Calculated Fermi surfaces of Ba₂CuO₂Fe₂As₂ using GGA relaxed parameters in the paramagnetic state.

0.15 holes per Fe atom. Considering the hole doping level, the Fermi surfaces attributed to Fe₂As₂ layers should be similar to Ba_{0.7}K_{0.3}Fe₂As₂ except that the pockets here are much more two-dimensional. This hole doping level is very close to that in optimally-hole-doped pnictide Ba_{0.6}K_{0.4}Fe₂As₂^{35–37} where T_c can reach 37 K. Actually, the calculated Fermi surfaces are similar to those of (Ba,K)Fe₂As₂ obtained in ARPES experiment^{38,39}. As required by the charge conservation, the heavy hole doping in Fe₂As₂ layers suggests that CuO₂ layers must be heavily electron-doped with the same doping concentration. This consistency is confirmed by the estimation that the size of the largest hole pocket at M point attributed to

$d_{x^2-y^2}$ orbitals in CuO_2 layers is about 0.3 electrons per Cu atom from their half filling configuration. The doping level is a little far from narrow superconducting region for electron-doped cuprates in the phase diagram¹⁴.

The superconductivity in both cuprates and IBS is mostly likely related to the magnetism. Therefore, we investigate the magnetic properties for this new compound. With such a large doping in the Fe_2As_2 and CuO_2 layers, it is expected that the checkerboard antiferromagnetic (AFM) order in the CuO_2 layers and the E-type collinear AFM order in Fe_2As_2 layers should be significantly weakened or completely suppressed even in the meanfield type of DFT calculations. To check this, we consider four possible magnetic states for Fe_2As_2 and CuO_2 layers: paramagnetic state, ferromagnetic state, checkerboard AFM state and collinear AFM state. We calculated the total energies of these magnetic states using the LDA+U approach. The calculations show that there is no statically ordered moment in CuO_2 layers while the E-type collinear AFM order in Fe_2As_2 layers is still possible. We find that in the DFT result, the E-type state has an energy gain of 103.5 meV/f.u. relative to the paramagnetic state and a spin moment of $1.59 \mu_B$ for each Fe. It is known that magnetic moments calculated on the known parent compounds of IBS, for example, BaFe_2As_2 , is typically over $2.0 \mu_B$ ^{33,40}. This moment value is significantly lowered, which is consistent with our expectation as Fe_2As_2 layers are overdoped by holes. Figure 5 (a) and (b) show the calculated band structure and DOS in the E-type collinear AFM state (with $\sqrt{2} \times \sqrt{2}$ supercell) with internal coordinates fixed to the values obtained by non-spin-polarized energy minimization. The E-type state is still metallic with low carrier concentration and $N(E_F)$ decreases severely. Among the considered magnetic states above, the checkerboard AFM state in Fe_2As_2 layers is found to be metastable state relative to the E-type collinear AFM state. The energy gain is 81.5 meV/f.u. relative to the paramagnetic state and the magnetic moment is about $1.58 \mu_B$ for each Fe atom.

With the substitution of As by Se and Ba by K in $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$, we obtain a new compound $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$. Compared with $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$, the parameter a decreases to 3.839 Å but c increases to 22.165 Å, which is consistent with those of iron chalcogenides. Table III lists the calculated lattice parameters using GGA and those of KFe_2Se_2 ¹³ and FeSe ⁴¹. The calculated Se height and Se-Fe-Se bond angle are very close to the values of FeSe , indicating that they may share some common electronic and magnetic properties. The Se heights are severely underestimated in the calculations compared with those in experiment⁴². The band structure and DOS are shown in Figure 6. The band structure is similar to that of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$. The DOS between -2.5 eV and 2.0 eV is dominated by Fe 3d states and Se 3p states are mainly located 3.5 eV below the Fermi level. The Cu 3d states and O 2p states are strongly coupled from -4.0 eV to 2.5 eV. The K atoms have no contribution to the bands near the Fermi level. To analyze the orbital characters near the Fermi level, we plot the fat band, shown in Figure 6(a). The DOS at the Fermi level is $4.54 \text{ eV}^{-1}/\text{f.u.}$, which is significantly lower than that of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$.

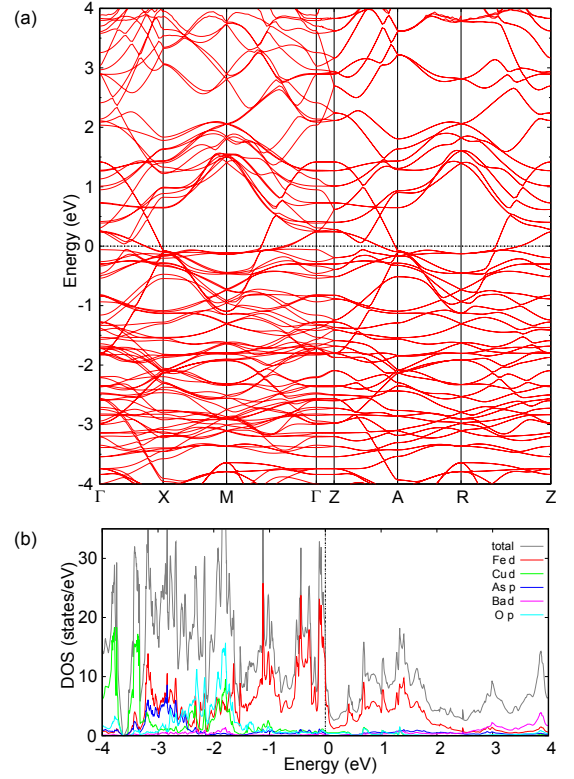


FIG. 5: (color online) Band structures and projected density of states of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ using GGA relaxed parameters in the E-type collinear AFM state.

TABLE III: Optimized structural parameters of $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$ using GGA in the paramagnetic phases and those of KFe_2Se_2 ¹³ and FeSe ⁴¹. The angle β is the Fe-Se-Fe bonding angle of two next nearest Fe atoms.

	$\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$	KFe_2Se_2	FeSe
$a(\text{\AA})$	3.839	3.913	3.765
$\beta(^{\circ})$	111.6	106.6	111.3
$h(\text{Fe-Se})(\text{\AA})$	1.31	1.46	1.29
$h(\text{Fe-Fe})(\text{\AA})$	11.08	7.02	5.52

The corresponding Pauli susceptibility and specific heat coefficient are $\chi_0 = 1.47 \times 10^{-4} \text{ emu/mol}$ and $\gamma = 10.7 \text{ mJ}/(K^2 \text{ mol})$. Figure 7 shows the calculated Fermi surfaces. The Fermi surfaces are two-dimensional cylinders. The Fe 3d states yield two hole pockets at Γ point and two small electron pockets at M point. The hole pockets are attributed to d_{xz} and d_{yz} states while the electron pockets are derived from Fe d_{xz} , d_{yz} and $d_{x^2-y^2}$ states. The Fermi surfaces are similar to those in KFe_2Se_2 where hole pockets are absent⁴³. Besides of pockets from Fe_2Se_2 layers, there are additional two hole pockets around the Brillouin zone corners. The bigger pocket is mainly contributed from Cu $d_{x^2-y^2}$ states, which are strongly coupled with the O p_x and p_y states, while the smaller one is derived from O p_x and p_y states. All of the Fermi surface sheets are double degenerate just as those in $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$.

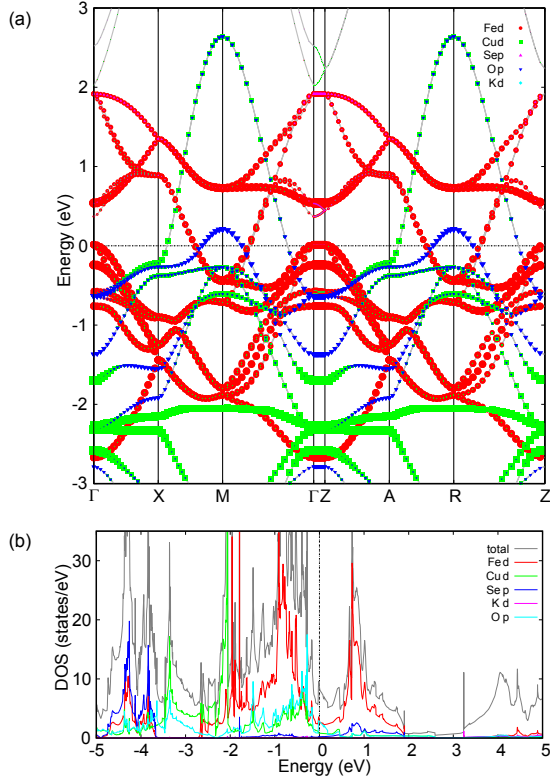


FIG. 6: (color online) Band structures and projected density of states of $K_2CuO_2Fe_2Se_2$ using GGA relaxed parameters in the paramagnetic state.

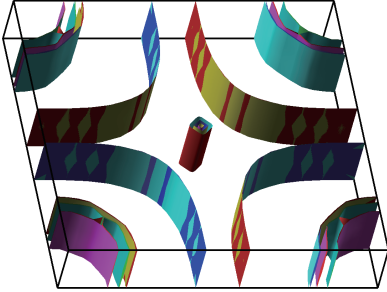


FIG. 7: (color online) Calculated Fermi surfaces of $K_2CuO_2Fe_2Se_2$ using GGA relaxed parameters in the paramagnetic state.

Compared with the Fermi surfaces of $Ba_2CuO_2Fe_2As_2$, we find that the hole pockets at Γ point of $K_2CuO_2Fe_2Se_2$ are much smaller while the electron pockets at M point are much larger (see Figure 7), which indicate heavy electron doping in the Fe_2Se_2 layer. From the size of the pockets, we can estimate that the electron doping concentration with respect to FeSe is roughly 0.16 electrons per Fe atom. Similarly, we can check the consistency required by the charge conservation. The size of the hole pockets at M point from CuO_2 layers is about 0.32 holes for each CuO_2 layer from their half filling configuration.

The DOS at the Fermi level attributed to Fe 3d orbitals is significantly decreased with such a large electron doping,

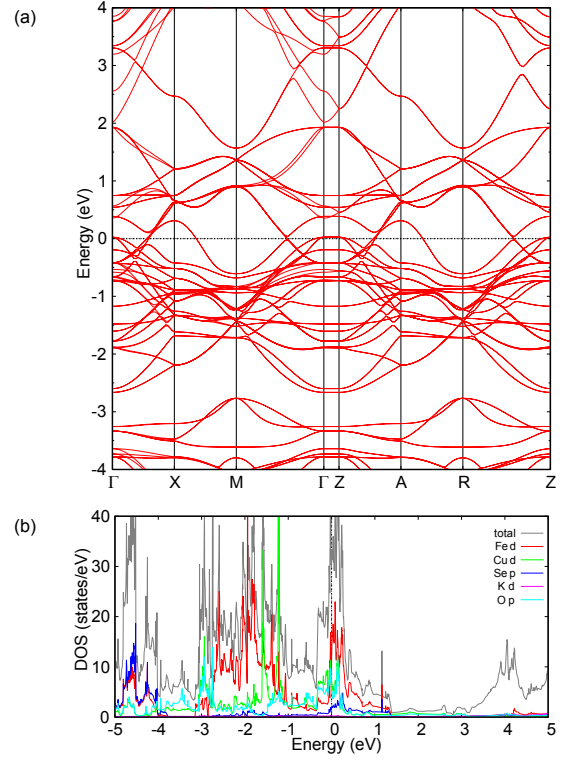


FIG. 8: (color online) Band structures and projected density of states of $K_2CuO_2Fe_2Se_2$ using GGA relaxed parameters in the AFM state.

which may suggest that magnetic order in Fe_2Se_2 layers is strongly suppressed. Compared with $Ba_2CuO_2Fe_2As_2$, we consider an additional bicollinear magnetic state, which is the ground state in FeTe⁴⁴. The ground state is paramagnetic on Fe_2Se_2 layers and checkboard AFM ordered for CuO_2 layers with a energy gain of 196.0 meV/f.u. and a spin moment of $0.59 \mu_B$ per Cu. The band structure and DOS are shown in Figure 8 and the system remains metallic. In this case, the Fe 3d, Cu 3d and O 2p states dominate the Fermi level. The DOS at the Fermi level is $7.04 \text{ eV}^{-1}/\text{f.u.}$ for spin up channel.

V. DISCUSSION

It is well known that the pairing symmetry is *d*-wave for the cuprates and *s*-wave for iron pnictides with a potential sign change between the hole and electron Fermi pockets. As the proposed new materials contain both CuO_2 layers and Fe_2X_2 ($X=As, Se$) layers and the electronic structures are similar to both, it can be expected that two different pairing symmetries may coexist in a single material. The proximity effect between two types of layers with different pairing symmetries can result in interesting novel phenomena. The time reversal symmetry may be broken with mixed *s*-wave and *d*-wave pairing symmetries.

Introducing additional carriers or applying external pressure in these materials can maximize T_c . For $Ba_2CuO_2Fe_2As_2$, the doping of Fe_2As_2 layer is 0.15 holes

per Fe and that of CuO_2 is 0.3 electrons per Cu. The doping for Fe_2As_2 layer is near the optimal level but that for CuO_2 layer is unfortunately not in the superconducting region. To realize superconductivity for both layers, we can introduce hole doping with partial replacement of Ba^{2+} ions by K^+ ions. From the phase diagrams of cuprates and $(\text{Ba},\text{K})\text{Fe}_2\text{As}_2$, the above case can be realized in $\text{Ba}_{2-x}\text{K}_x\text{CuO}_2\text{Fe}_2\text{As}_2$ ($0.24 \leq x \leq 0.32$) by assuming that the Fe_2As_2 and CuO_2 layers are equally hole doped. In this doping region, the T_c for Fe_2As_2 layers shows little change. $x = 0.3$ corresponds the optimal doping value for electron-doped cuprates¹⁴. For $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$, however, the Fe_2Se_2 layers are electron doped and the hole doping for CuO_2 layers is not in superconducting region but very close to it. The superconductivity for both layers can be realized in $\text{K}_{2-x}\text{Ba}_x\text{CuO}_2\text{Fe}_2\text{Se}_2$ ($0.10 \leq x \leq 0.54$). This doping region is much wider than that in $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ due to the wide hole-doped superconducting region in cuprates. The optimal doping value for CuO_2 layers is $x = 0.34$. The pressure is also an effective way to tune the superconductivity.

VI. CONCLUSION

In conclusion, we identify two hypothetical compounds $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ and $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$ containing Fe_2X_2 layers and CuO_2 layers, which are the basic structural units of

IBS and cuprates, respectively. The metallic spacer $\text{Ba}(\text{K})$ separates the basic units. The calculations of binding energies and phonon spectrums indicate that they are dynamically stable, ensuring that they may be experimentally synthesized. The Fermi surfaces derived from $\text{Fe}_2\text{As}_2(\text{Fe}_2\text{Se}_2)$ layers and CuO_2 layers are very similar to those of iron pnictides (iron chalcogenides) and cuprates, respectively. With heavy self-doping, the ground state of $\text{Ba}_2\text{CuO}_2\text{Fe}_2\text{As}_2$ is determined to be E-type collinear AFM state in the Fe_2As_2 layer and paramagnetic state in the CuO_2 layer, while $\text{K}_2\text{CuO}_2\text{Fe}_2\text{Se}_2$ favors checkboard AFM state in CuO_2 layers and paramagnetic state in Fe_2Se_2 layers. Without external doping, superconductivity can only be achieved in Fe_2X_2 layers. However, with external doping through substitution, superconductivity for both Fe_2X_2 and CuO_2 layers can be simultaneously achieved in $\text{Ba}_{2-x}\text{K}_x\text{CuO}_2\text{Fe}_2\text{As}_2$ ($0.24 \leq x \leq 0.32$) and $\text{K}_{2-x}\text{Ba}_x\text{CuO}_2\text{Fe}_2\text{Se}_2$ ($0.10 \leq x \leq 0.54$). The synthesis of these new compounds will not only provide us a unique opportunity to explore exotic properties in cuprates and IBS simultaneously but also help us to understand the mechanism of high T_c superconductivity.

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